

Arizona Chemical Company
December 2005

Robust Summaries of Existing Data for CASRN 71243-68-0 (corrected to CASRN 258342-84-6)

PHYSICO-CHEMICAL PROPERTY – BOILING POINT	
<u>Test Substance</u>	
Chemical Name	Resin acids and Rosin acids, fumarated, decyl esters
CASRN	71243-68-0 (corrected to CASRN 258342-84-6)
<u>Method</u>	
Method/Guideline followed	Tested according to distillation method based on ISO 918:1983, Method 103 of the OECD Guidelines for the Testing of Chemicals, 12 May 1981.
Test Type	Boiling temperature
GLP (Y/N)	Y
Year (Study Performed)	1996
Test Conditions	<p>Distillation at atmospheric pressure: An aliquot (50.9 g) of test material was placed in a round-bottomed flask and the flask connected to a condenser and collection vessel. In order to measure the vapor recondensation temperature, a thermometer was secured in the neck of the flask. An additional thermometer was immersed in the test material in order to measure the sample temperature. The flask was heated steadily by means of a heating mantle. The appearance of the test material and the amount of distillate produced during the test were monitored. On concluding the test the atmospheric pressure was measured using a Fortins barometer.</p> <p>Distillation at reduced pressure: Same as above except system pressure was reduced by means of a vacuum pump and the pressure monitored using a mercury manometer.</p>
<u>Results</u>	Boiled with decomposition over the range approximately 557 to 630 \pm 0.5°K at an atmospheric pressure of 102.18 kPa. Boiled with decomposition over the range approximately 551 to 604 \pm 0.5°K at a reduced pressure of 0.8 to 2.9 kPa.
<u>Data Quality</u>	Reliable without restrictions – Klimisch Code 1a
<u>References</u>	Hogg, A.S.; Bartlett, A.J. 1996. Determination of General Physico-Chemical Properties SPL Project Number 874/001, SafePharm Laboratories Limited, Derby, United Kingdom.

PHYSICO-CHEMICAL PROPERTY – POUR POINT	
<u>Test Substance</u>	
Chemical Name	Resin acids and Rosin acids, fumarated, decyl esters
CASRN	71243-68-0 (corrected to CASRN 258342-84-6)
<u>Method</u>	
Method/Guideline followed	Tested according to BS 2000 Part 15:1982, Method 102 of the OECD Guidelines for the Testing of Chemicals, 12 May 1981.
Test Type	Pour point
GLP (Y/N)	Y
Year (Study Performed)	1996
Test Conditions	Test material was placed in a jar of dimensions approx. 120 mm height, 32 mm internal diameter and 53 mm fill height. Test jar was fitted with a glass jacket resulting in a 5 mm air gap around the jar. The sample was equilibrated at approx. 48°C before being allowed to cool to 35°C. The sample was then cooled in an ice batch maintained at -1 to 2°C. At 3°C intervals, the test jar was removed and tilted to a horizontal position for a period of 5 seconds; this was continued until the sample was observed to remain stationary.
<u>Results</u>	The pour point was determined to be $285 \pm 3^{\circ}\text{K}$.
<u>Data Quality</u>	Reliable without restrictions – Klimisch Code 1a
<u>References</u>	Hogg, A.S.; Bartlett, A.J. 1996. Determination of General Physico-Chemical Properties SPL Project Number 874/001, SafePharm Laboratories Limited, Derby, United Kingdom.

PHYSICO-CHEMICAL PROPERTY – VAPOR PRESSURE	
<u>Test Substance</u>	
Chemical Name	Resin acids and Rosin acids, fumarated, decyl esters
CASRN	71243-68-0 (corrected to CASRN 258342-84-6)
<u>Method</u>	
Method/Guideline followed	Tested according to Method 104 of OECD Guidelines for the Testing of Chemicals, 12 May 1981.
Test Type	Vapor pressure
GLP (Y/N)	Y
Year (Study Performed)	1996
Test Conditions	<p>The vapor pressure was determined using a vapor pressure balance based on a CI Electronics microbalance with a sensitivity of approx. 0.1 μg. The temperature of the sample was controlled electronically. The mass and temperature readings were recorded automatically into a computer file.</p> <p>After evacuating the system, opening the shutter above the sample oven causes the escaping vapor jet to be directed at the scale pan. The difference in mass readings with the orifice covered and uncovered is proportional to the vapor pressure at the given oven temperature.</p> <p>Four runs were done. Run 4 was chosen because the sample had been under vacuum for the longest period prior to the run and so degassing would have been the most complete.</p>
<u>Results</u>	Vapor pressure determined to be less than 9.4×10^{-4} Pa at 25°C.
<u>Data Quality</u>	Reliable without restrictions – Klimisch Code 1a
<u>References</u>	Tremain, S.P.; Bartlett, A.J. 1996. Determination of Vapour Pressure SPL Project Number 874/002, SafePharm Laboratories Limited, Derby, United Kingdom.

PHYSICO-CHEMICAL PROPERTY – RELATIVE DENSITY	
<u>Test Substance</u>	
Chemical Name	Resin acids and Rosin acids, fumarated, decyl esters
CASRN	71243-68-0 (corrected to CASRN 258342-84-6)
<u>Method</u>	
Method/Guideline followed	Tested using the pycnometer, Method 109 of the OECD Guidelines for the Testing of Chemicals, 12 May 1981.
Test Type	Density
GLP (Y/N)	Y
Year (Study Performed)	1996
Test Conditions	A pycnometer of 30 ml nominal capacity was cleaned and dried to constant mass. A calibration was carried out by determining the mass of distilled water (equilibrated to $20 \pm 0.5^{\circ}\text{C}$) required to fill the pycnometer. The pycnometer was again dried to constant mass, then filled with test material which had been warmed to $50 \pm 0.5^{\circ}\text{C}$. The pycnometer and test material were equilibrated to $20 \pm 0.5^{\circ}\text{C}$ and the mass of the pycnometer filled with test material measured. Duplicates were run.
<u>Results</u>	The density was determined to be 1014.4 kg/m^3 at $20.5 \pm 0.5^{\circ}\text{C}$.
<u>Data Quality</u>	Reliable without restrictions – Klimisch Code 1a
<u>References</u>	Hogg, A.S.; Bartlett, A.J. 1996. Determination of General Physico-Chemical Properties SPL Project Number 874/001, SafePharm Laboratories Limited, Derby, United Kingdom.

PHYSICO-CHEMICAL PROPERTY – WATER SOLUBILITY	
<u>Test Substance</u>	
Chemical Name	Resin acids and Rosin acids, fumarated, decyl esters
CASRN	71243-68-0 (corrected to CASRN 258342-84-6)
<u>Method</u>	
Method/Guideline followed	Tested according to the flask method, Method 105 of the OECD Guidelines for the Testing of Chemicals, 12 May 1981.
Test Type	Water solubility
GLP (Y/N)	Y
Year (Study Performed)	1996
Test Conditions	<p>A preliminary test was carried out to determine the approximate water solubility. Based on the preliminary result, weighed 0.17 g of test material into a flask and added 150 ml of glass double-distilled water. Samples were prepared in triplicate. Flasks were shaken at approx. 30°C (sample 1 – 25.5 hrs; sample 2 – 49.5 hrs; sample 3 – 73.5 hrs). At end of shaking, flasks were left to stand at 20°C for a period of 24 hours. The pH of each sample solution was measured. The contents of the flasks were filtered and the concentrations determined by high performance liquid chromatography (HPLC). An aliquot (100 ml) was extracted with three portions (3 X 25 ml) of dichloromethane, each extract being filtered through anhydrous sodium sulfate. The combined extracts were then evaporated to dryness and the residue re-dissolved in 2.0 ml of methanol. Duplicate standard solutions were prepared in methanol at a nominal concentration of 200 mg/l.</p> <p>The preliminary test indicated the column elution method should have been performed as the solubility was less than 1×10^{-2} g/l. However, due to the physical nature of the material, it was not possible to perform the test without blocking the column. The test material and beads adhere together, forming a plug within the column and thus preventing water circulation.</p>
<u>Results</u>	Water solubility was determined to be $<3.45 \times 10^{-4}$ g/l of solution at $20.0 \pm 0.5^\circ\text{C}$.
<u>Data Quality</u>	Reliable without restrictions – Klimisch Code 1a
<u>References</u>	Hogg, A.S.; Bartlett, A.J. 1996. Determination of General Physico-Chemical Properties SPL Project Number 874/001, SafePharm Laboratories Limited, Derby, United Kingdom.

PHYSICO-CHEMICAL PROPERTY – PARTITION COEFFICIENT	
<u>Test Substance</u>	
Chemical Name	Resin acids and Rosin acids, fumarated, decyl esters
CASRN	71243-68-0 (corrected to CASRN 258342-84-6)
<u>Method</u>	
Method/Guideline followed	Tested according to shake-flask method, Method 107 of the OECD Guidelines for the Testing of Chemicals, 12 May 1995.
Test Type	Partition coefficient
GLP (Y/N)	Y
Year (Study Performed)	1996
Test Conditions	<p>A preliminary assessment of partition coefficient was determined based on the approx. solubilities of the test material in n-octanol and distilled water.</p> <p>A stock solution was prepared by diluting an aliquot (27.3 g) of test material to 2000 ml with water saturated n-octanol. Six partitions were performed. The shaking was performed by inversion of the flasks through approx. 180° over a five minute period. After separation, aliquots of both phases were taken for analysis. The concentration of the sample solutions was determined spectrophotometrically. The organic phase samples were diluted by a factor of 625 using acetonitrile. Duplicate aliquots of stock solution were diluted by a factor of 625 using acetonitrile. Duplicate standard solutions were prepared in acetonitrile at a nominal concentration of 20 mg/l.</p> <p>An aliquot (100 ml) of aqueous phase samples was extracted with three portions (3 x 25ml) of dichloromethane, each extract being filtered through anhydrous sodium sulfate. The combined extracts were then evaporated to dryness and the residue dissolved in acetonitrile (25 ml).</p> <p>The absorbance of the standard, sample and stock solutions was measures at 220 nm in cells of 10 mm path length using acetonitrile as the reference medium.</p>
<u>Results</u>	Partition coefficient has been determined to be greater than 2.15×10^3 at $22.0 \pm 0.5^\circ\text{C}$; $\text{Log}_{10}\text{P}_{\text{OW}} = > 3.33$
<u>Data Quality</u>	Reliable without restrictions – Klimisch Code 1a
<u>References</u>	Hogg, A.S.; Bartlett, A.J. 1996. Determination of General Physico-Chemical Properties SPL Project Number 874/001, SafePharm Laboratories Limited, Derby, United Kingdom.

ACUTE TOXICITY-ORAL	
<u>Test Substance</u>	
Chemical Name	Resin acids and Rosin acids, fumarated, decyl esters
CASRN	71243-68-0 (corrected to CASRN 258342-84-6)
<u>Method</u>	
Method/Guideline followed	Similar to OECD Guideline 401, "Acute Oral Toxicity."
GLP (Y/N)	Y
Year (Study Performed)	1995
Species	Rat
Strain	Sprague-Dawley
Route of Administration	Oral
Dose levels	5,000 mg/kg, single dose
Sex and number/group	10 per group; 5 Male; 5 Female
Frequency of treatment	Single oral gavage
Duration of test	14 day observation post-treatment
Control group (Y/N)	N
<u>Result</u>	
Acute Oral LD ₅₀	Greater than 5,000 mg/kg in rats when administered as a 75% w/w solution in corn oil.
<u>Detailed Summary</u>	
	<p>Ten (five male and five female) healthy albino Sprague-Dawley rats received a single oral (gavage) dose of 5,000 mg/kg of the test material administered as a 75% w/w solution in corn oil. Animals were weighed initially and on days 7 and 14. Animals were observed for signs of gross toxicity and behavioral changes at 0.25, 2 and 3 hrs post-dosing and at least once daily for 14 days. Parameters evaluated included gross evaluation of skin and fur, eyes and mucous membranes, respiratory, circulatory, autonomic and central nervous systems, somatomotor activity, behavior pattern, mortality, body weight and gross pathology. Particular attention was directed to observation of tremors, convulsions, salivation, diarrhea and coma. No deaths occurred and all 10 animals gained weight. One female exhibited soft feces between 2 and 3 hours after test article administration. All other animals appeared active and healthy. There were no signs of gross toxicity, adverse pharmacologic effects or abnormal behavior. Gross necropsy findings at terminal sacrifice were generally unremarkable.</p>
<u>Data Quality</u>	
Reliable without restrictions – Klimisch Code 1a	
<u>References</u>	
Wnorowski, G. 1995. Acute oral toxicity limit test of [trade name deleted; C9-11 isoalkyl, C10-rich ester of fumarated rosin] in the rat. Study No. 3977. Product Safety Labs, East Brunswick, New Jersey.	

ACUTE TOXICITY - DERMAL	
<u>Test Substance</u>	
Chemical Name	Resin acids and Rosin acids, fumarated, decyl esters
CASRN	71243-68-0 (corrected to CASRN 258342-84-6)
<u>Method</u>	
Method/Guideline followed	Similar to OECD Guideline 402, "Acute Dermal Toxicity."
GLP (Y/N)	Y
Year (Study Performed)	1995
Species	Rat
Strain	Sprague-Dawley
Route of Administration	Dermal
Dose levels	5,000 mg/kg, single dose
Sex and number/group	10 per group; 5 Male; 5 Female
Frequency of treatment	Single dermal administration to area 2" x 3" (10% of body surface) covered with gauze patch.
Duration of test	14 day observation post-treatment
Control group (Y/N)	N
<u>Result</u>	
Acute Oral LD ₅₀	Greater than 5,000 mg/kg in rats when administered at 100% concentration.
<u>Detailed Summary</u>	
	Ten (five male and five female) healthy albino Sprague-Dawley rats received a single dose of 5,000 mg/kg of the test material administered at 100% conc. as received applied to a 2" x 3" clipped patch of skin (approx. 10% of the body surface) and covered with an adhesive-backed gauze patch. After 24 hrs. exposure, the patches were removed and the test sites wiped to remove any residual test material. Animals were weighed initially and on days 7 and 14. Animals were observed for signs of gross toxicity and behavioral changes at 1 and 5 hours after application and at least once daily for 14 days. Parameters evaluated included gross evaluation of skin and fur, eyes and mucous membranes, respiratory, circulatory, autonomic and central nervous systems, somatomotor activity, behavior pattern, mortality, body weight and gross pathology. All animals survived, gained weight and appeared active and healthy. There were no signs of gross toxicity, adverse pharmacologic effects or abnormal behavior. Gross necropsy findings at terminal sacrifice revealed dark foci on the lungs of one male. Otherwise, necropsy findings were generally unremarkable.
<u>Data Quality</u>	
	Reliable without restrictions – Klimisch Code 1a
<u>References</u>	
	Wnorowski, G. 1995. Acute dermal toxicity limit test in the rat. Study No. 3978. Product Safety Labs, East Brunswick, New Jersey.

IN VITRO GENETIC TOXOCITY-MUTATION	
<u>Test Substance</u>	
Chemical Name	Resin acids and Rosin acids, fumarated, decyl esters
CASRN	71243-68-0 (corrected to CASRN 258342-84-6)
<u>Method</u>	
Method/Guideline followed	OECD Method 471, "Bacterial Reverse Mutation Test"
GLP (Y/N)	Y
Year (Study Performed)	1995
System of testing	<i>s. typhimurium</i> strains TA98, TA100, TA1535 and TA1537 <i>E. coli</i> WP2uvrA
Concentration	250, 500, 1000, 2500 and 5000 µg/plate
Metabolic activation	With and without addition of Arochlor 1254-induced rat liver S-9
<u>Results</u>	Non-mutagenic with or without metabolic activation
<u>Detailed Summary</u>	<p>Material was tested for its potential to cause mutation at the histidine operon of in <i>S. typhimurium</i> strains TA98, TA100, TA1535 and TA1537 and at the tryptophan operon of <i>E. coli</i> strain WP2uvrA. The first Mutation Assay, using the plate incorporation method, was performed with the four <i>S. typhimurium</i> tester strains and the <i>E. coli</i> strain using concentrations of 250, 500, 1000, 2500 and 5000 µg/plate with and without metabolic activation with S9 fraction from Aroclor 1254-treated Sprague-Dawley rats. The second Mutation Assay, using the preincubation method, was performed to confirm the results of the first assay using the same concentrations. Positive controls not requiring metabolic activation included: 2-nitrofluorene, sodium azide, 9-aminoacridine and methyl methanesulfonate. The positive control requiring metabolic activation was 2-aminoanthracene. All test concentrations, including the controls, were tested in triplicate.</p> <p>In the non-activated system of the confirmatory assay, <i>Salmonella</i> strain TA100 showed signs of slight toxicity at the highest test article concentration of 5000 µg/plate. All of the lower concentrations had a similar number of revertants as in the corresponding solvent controls, and there was no dose-related response in either system. There were no signs of toxicity in the <i>E. coli</i> strain. Thus, the test article produced a negative response.</p> <p>The results of both Mutation Assays indicated that the test article did not induce any positive increase in the number of revertant colonies for any of the tester strains in the</p>

	<p>presence or absence of Aroclor 1254-induced rat liver S-9.</p> <p>Under conditions of the study, the test article is negative in the <i>Salmonella typhimurium</i>/<i>Escherichia coli</i> Plate Incorporation/Preincubation Mutation Assay.</p>
<u>Data Quality</u>	Reliable without restrictions – Klimisch Code 1a
<u>References</u>	<p>Pant, Kamala J. 1995. Evaluation of a Test Article in the <i>Salmonella typhimurium</i>/<i>Escherichia coli</i> Plate Incorporation/Preincubation Mutation Assay in the Presence and Absence of Aroclor-Induced Rat Liver S-9 With a Confirmatory Study. Study No. 0367-2140. SITEK Research Laboratories, Rockville, Maryland.</p>